

GPT-one-hot

GPT

one-hot Tanimoto

drfp RBF

drfp linear

rxnfp RBF

rxnfp linear

accuracy

F₁ macroF₁ micro κ

0.4

0.2

0.2

0.4

0.2

0.2

0.0

25

50

75

100

125

150

175

200